IFP
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5. Übung QFT für Vielteilchen-Systeme

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Consider the Hubbard-Hamiltonian given by

$$\hat{\mathcal{H}} = \sum_{\mathbf{k}\sigma} \varepsilon_{\mathbf{k}} \hat{c}_{\mathbf{k}\sigma} \hat{c}^\dagger_{\mathbf{k}\sigma} + U \sum_i \underbrace{\hat{c}^\dagger_{i\uparrow}\hat{c}_{i\uparrow}}_{\hat{n}_{i\uparrow}} \underbrace{\hat{c}^\dagger_{i\downarrow}\hat{c}_{i\downarrow}}_{\hat{n}_{i\downarrow}} - \mu \sum_i \underbrace{(n_{i\uparrow} + n_{i\downarrow})}_{\hat{n}_i}. \tag{1}$$

The term containing μ fixes the number of particles. Specifically, here we consider the case of half-filling where we have $\langle \hat{n}_i \rangle = 1$ particles/site. This corresponds to $\boldsymbol{\mu = \frac{U}{2}}$.

1. The Green's function of a free-particle-system *4+2+1=7 Punkte*

First, assume that the electrons are non-interacting, i.e., $\boldsymbol{U = 0}$.

a) Calculate the one-particle Green's function $G_\sigma(\tau, \mathbf{k})$ by directly calculating the trace in the definition

$$G_\sigma(\tau, \mathbf{k}) = -\frac{1}{\mathcal{Z}} \mathrm{Tr}\left[e^{-\beta \hat{\mathcal{H}}} \hat{c}_{\mathbf{k}\sigma}(\tau) \hat{c}^\dagger_{\mathbf{k}\sigma} \right], \quad \beta \geq \tau \geq 0 \tag{2}$$

of the Green's function. (The partition function is defined as $\mathcal{Z} = \mathrm{Tr}[e^{-\beta\hat{\mathcal{H}}}]$.)
Hint: Consider the equation of motion for the operator $\hat{c}_{\mathbf{k}\sigma}(\tau)$, i.e.,

$$\frac{\partial}{\partial \tau} \hat{c}_{\mathbf{k}\sigma}(\tau) = [\hat{\mathcal{H}}, \hat{c}_{\mathbf{k}\sigma}(\tau)] = e^{\tau\hat{\mathcal{H}}} [\hat{\mathcal{H}}, \hat{c}_{\mathbf{k}\sigma}] e^{-\tau\hat{\mathcal{H}}}. \tag{3}$$

Solve this differential equation (for the case $U = 0$) to find an expression for $\hat{c}_{\mathbf{k}\sigma}(\tau)$.

b) Calculate the Green's function $G_\sigma(i\omega_n, \mathbf{k})$ in frequency space by performing the Fourier-transform

$$G_\sigma(i\omega_n, \mathbf{k}) = \int_0^\beta d\tau \; e^{i\omega_n \tau} G_\sigma(\tau, \mathbf{k}), \tag{4}$$

where $\omega_n = \frac{\pi}{\beta}(2n+1)$, $n \in \mathbb{Z}$ is a fermionic Matsubara-frequency.

c) Continue the result obtained in 1a) for $G_\sigma(\tau, \mathbf{k})$ to real times by the inverse Wick-rotation $\tau \to it$. Give a physical interpretation for the result.

2. The Green's function for the atomic limit *4+2=6 Punkte*

Now, consider the opposite limit where the kinetic energy is negligible compared to the interaction, i.e., $\varepsilon_{\mathbf{k}} = 0$.

a) Compute the (local!) Green's function for site i, $G_{i\sigma}(\tau)$, defined as

$$G_{i\sigma}(\tau) = -\frac{1}{\mathcal{Z}} \mathrm{Tr}\left[e^{-\beta \hat{\mathcal{H}}} \hat{c}_{i\sigma}(\tau) \hat{c}^\dagger_{i\sigma} \right], \quad \beta \geq \tau \geq 0 \tag{5}$$

by directly evaluating the trace.
Hint: Consider that the different atoms are completely independent and hence, one can evaluate the trace by using the occupation-basis for one site, which consists of four states. Which are these?

b) Calculate the Green's function $G_{i\sigma}(i\omega_n)$ in frequency-space by performing the Fourier transform for the result obtained in 2a).